

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 306 °C

Global applicability domain: Inside

Local applicability domain index: 2.72e-01

Confidence level: 5.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>3-Nitrobenzamide</div> <div>Measured: 313</div> <div>Predicted: 310</div>	<div>Image not found</div> <div>2-Nitrobenzamide</div> <div>Measured: 317</div> <div>Predicted: 310</div>	<div>Image not found</div> <div>Phenacetin</div> <div>Measured: 244</div> <div>Predicted: 301</div>
<div>Image not found</div> <div>Propanil</div> <div>Measured: 351</div> <div>Predicted: 317</div>	<div>Image not found</div> <div>3,3-dimethylindolin-2-one</div> <div>Measured: 300</div> <div>Predicted: 290</div>	